Glycine ethyl ester

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Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.93	22.5	0.93	22.1	0.93	22.1	

Model Results

Predicted value: 150 °C

Global applicability domain: Inside

Local applicability domain index: 6.01e-01

Confidence level: 6.95e-01

Nearest Neighbors from the Training Set

Image not found

Glycine ethyl ester Measured: 149 Predicted: 150

Image not found

2,2-

Dimethoxyethyl(methyl)amine

Measured: 140 Predicted: 135

Image not found

2-Pentanone, 4-amino-4-methyl-

Measured: 180 Predicted: 171

Image not found

Morpholine
Measured: 128
Predicted: 117